Renormalization algorithms for Quantum-Many Body Systems in two and higher dimensions

F. Verstraete and J. I. Cirac
Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, Garching, D-85748, Germany.
(Dated: February 2, 2008)

We describe quantum many–body systems in terms of projected entangled–pair states, which naturally extend matrix product states to two and more dimensions. We present an algorithm to determine correlation functions in an efficient way. We use this result to build powerful numerical simulation techniques to describe the ground state, finite temperature, and evolution of spin systems in two and higher dimensions.

PACS numbers: PACS

The theoretical investigation of strongly correlated systems is one the most challenging tasks in several fields of Physics. Even though several analytical techniques and numerical methods have been developed during the last decades, there still exist a rich variety of systems which remain untractable. Even some of the simplest systems, which deal with spins in lattices with short range interactions, are very hard to simulate numerically. The development of powerful numerical techniques would allow us to discover a rich variety of intriguing phenomena and to confirm some of the predictions which have been made.

In the case of 1D systems, much analytical insight has been gained by finding exact expressions for the ground and/or excited eigenstates of some particular Hamiltonians, as it is the case for the 1D–AKLT states [1]. On the other hand, a very powerful numerical simulation method known as DMRG [2] has allowed us to determine physical properties of generic spin chains to an unprecedented accuracy. Recent work has also shown how DMRG can be adapted to simulate the spin dynamics at zero-temperature [3] or at finite temperature and in the presence of dissipation [4, 5]. The success of the DMRG method and its extensions relies on the existence of the so-called matrix product states (MPS) [6], which generalize the 1D–AKLT states. The DMRG method can be understood as a variational method within these MPS [7, 8, 9], and part of its success relays on the fact that correlation functions can be efficiently calculated.

In two or higher dimensions, however, almost no models have been solved exactly. A generalization of DMRG to higher dimensions is hard to scale, as the MPS–ansatz explicitly assumes a 1D configuration. The Monte Carlo method [10], on the other hand, is very useful to describe certain systems, but for models with frustration is, unlike DMRG, plagued by the so-called sign problem. The physics of 2D spin systems is therefore not very well understood as compared to 1D systems; this is very unfortunate as a good understanding would shed new light on many open questions in condensed matter, such as high-T_c superconductivity.

In this paper, we present a natural generalization of the 1D MPS to two and higher dimensions and build simulation techniques based on those states which effectively extend DMRG to higher dimensions. We call those states *projected entangled–pair states* (PEPS), since they can be understood in terms of pairs of maximally entangled states of some auxiliary systems, and that are projected in some low–dimensional subspaces locally. This class of states includes the generalizations of the 2D AKLT-states known as tensor product states [11] which have been used for 2D problems (see also [12, 13, 14]) but is much broader since every state can be represented as a PEPS (as long as the dimension of the entangled pairs is large enough). We also develop an efficient algorithm to calculate correlation functions of these PEPS, and which allows us to extend the 1D algorithms [2, 3, 4, 5] to higher dimensions. This leads to many interesting applications, such as scalable variational methods for finding ground or thermal states of spin systems in higher dimensions as well as to simulate their time-evolution. For the sake of simplicity, we will present our results for a square lattice in 2D, but they are easily generalized to higher dimensions and other geometries.

Let us start by recalling the representation introduced in [9] of the state Ψ of N d–dimensional systems in terms of MPS. For that, we substitute each physical system k by two auxiliary systems a_k and b_k of dimension D (except at the extremes of the chain). Systems b_k and a_{k+1} are in a maximally entangled state $|\phi\rangle = \sum_{n=1}^{D} |n,n\rangle$, which is represented in Fig. 1(a) by a solid line (bond) joining them. The state Ψ is obtained by applying a linear operator Q_k to each pair a_k, b_k that maps the auxiliary systems onto the physical systems, i.e.

$$\begin{aligned} |\Psi\rangle &= Q_1 \otimes Q_2 \otimes \dots Q_N \ |\phi\rangle \dots |\phi\rangle \\ &= \sum_{s_1,\dots,s_N=1}^{d} \mathrm{F}_1(A_1^{s_1},\dots,A_N^{s_N})|s_1,\dots,s_N\rangle, \quad (1) \end{aligned}$$

where the matrices A_k^s have elements $(A_k^s)_{l,r} = \langle s|Q_k|l,r\rangle$. Note that the indices l and r of each matrix A_k^s are related to the left and right bonds of the auxiliary systems with their neighbors, whereas the index s denotes the state of the physical system. The function F_1 is just the trace of the product of the matrices, i.e. it

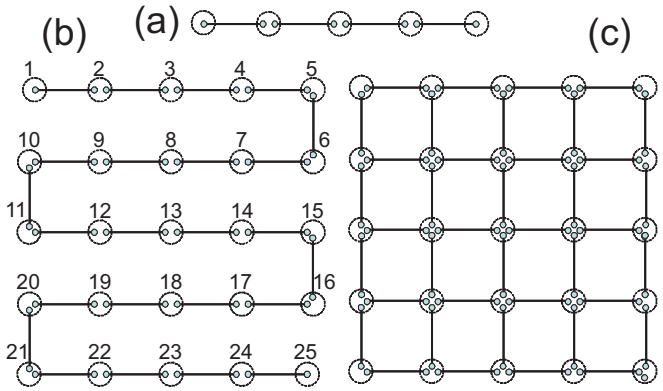

FIG. 1: Graphical representation of MPS in 1 dimension (a), in 2 dimensions (b), and of PEPS (c). The bonds represent pairs of maximally entangled D–dimensional auxiliary spins and the circles denote projectors that map the inner auxiliary spins to the physical ones.

contracts the indices l, r of the matrices A according to the bonds.

As shown in [9], every state can be represented in the form (1) as long as the dimension D can be chosen sufficiently large. Note, however, that the above picture of the state is basically one dimensional, since each auxiliary system is entangled only to one nearest neighbor. Thus, these states appear to be better suited to describe 1D systems, with short range interactions, since a small local dimension D may give a good approximation to the real state of the whole system. Note also that, as it is clear from the above representation, any block of systems is only entangled to the rest by at most two maximally entangled state of the auxiliary particles and thus its entropy is bounded by $2\log_2 D$, independent of the block size. This has been identified as the main reason why DMRG does not describe well critical systems, where the entropy grows with the logarithm of the block size [15].

States in the form (1) have also been used to represent 2D systems [16]. For simplicity let us thus consider a 2D square lattice of $N := N_h \times N_v$ systems. The idea there is to numerate them in such a way that they can be regarded as a long 1D system [Fig. 1(b)]. In general, this method cannot be extended to larger systems since nearest neighbor interactions in the original 2D system (for example between 11 and 20) give rise to long interactions in the effective 1D description. Moreover, the entropy of some blocks does not scale as the area of the block, as it is expected for 2D configurations. For example, the block formed by systems from 6–15 has at most a constant entropy of $2\log_2 D$.

For 2D systems we propose to use the description based on Fig. 1(c). Each physical system of coordinates (h, v) is represented by four auxiliary systems $a_{h,v}$, $b_{h,v}$, $c_{h,v}$, and $d_{h,v}$ of dimension D (except at the borders of the lattices). Each of those systems is in a maximally entangled state ϕ with one of its neighbor, as shown in the figure. The state Ψ is obtained by applying to each site one operator $Q_{h,v}$ that maps the auxiliary systems onto the physical systems:

$$|\Psi\rangle = \sum_{s_{1,1},\ldots,s_{N_h,N_v}=1}^{d} \mathrm{F}_2(\{A_{h,v}^{s_{h,v}}\})|s_{1,1},\ldots,s_{N_h,N_v}\rangle. \quad (2)$$

Here, the A's are four index tensors with elements $(A^s_{h,v})_{u,d,l,r} = \langle s|Q_{h,v}|u,d,l,r\rangle$. As in the 1D case, we associate each index of such tensors to each direction (up, down, left, and right). Thus, the position with coordinates (h, v) is represented by a tensor $(A^s_{h,v})_{u,d,l,r}$ whose index s is represents the physical system, and the other four indices are associated with the bonds between the auxiliary systems and the neighboring ones. The function F_2 contracts all these indices u, d, l, r of all tensors A according to those bonds. Note that we can generalize this construction to any lattice shape and dimension, and that using the construction of [9] one can show that any state can be written as a PEPS. In this way, we also resolve the problem of the entropy of blocks mentioned above, since now this entropy is proportional to the bonds that connect such block with the rest, and therefore to the area of the block. Note also that, in analogy to the MPS [6], the PEPS are guaranteed to be ground states of local Hamiltonians.

We show now how to determine expectation values of operators in the state Ψ (2). We consider a general operator $O = \prod_{h,c} O_{h,c}$ and define the four–indices tensor

$$(E_{O_{h,c}})_{\tilde{u},\tilde{d},\tilde{l},\tilde{r}} := \sum_{s,s'=1}^{d} \langle s|O_{h,c}|s'\rangle (A^s)_{u,d,l,r} (A^{s'})^*_{u',d',l',r'} \quad (3)$$

where the indices are combined in pairs, i.e., $\tilde{u} = (u, u')$, $\tilde{d} = (d, d')$, $\tilde{l} = (l, l')$, and $\tilde{r} = (r, r')$. One can easily show that $\langle\Psi|O|\Psi\rangle = \mathrm{F}_2(E_{O_{h,c}})$. Thus, the evaluation of expectation values consists of contracting indices of the tensors E. In order to show how to do this in practice, we notice that the tensors associated to the first and last rows, once contracted, can be reexpressed in terms of a MPS. In particular, we define [compare (1)]

$$|U_1\rangle := \sum_{d_1\ldots d_N=1}^{D^2} \mathrm{F}_1(E^{d_1}_{1,1}\ldots E^{d_N}_{1,N})|d_1\ldots d_N\rangle, \quad (4a)$$

$$\langle U_{N_v}| := \sum_{u_1\ldots u_N=1}^{D^2} \mathrm{F}_1(E^{u_1}_{N,1}\ldots E^{u_N}_{N,N})\langle u_1\ldots u_N|. \quad (4b)$$

Here we have used the short–hand notation $E_{h,c} := E_{O_{h,c}}$, and the fact that the tensors in the first and last rows have at most three indices [see Fig. 1c]. Thus, the horizontal indices (l, r) of the tensors play the role of the indices of each matrix, whereas the vertical ones (d) plays

the role of the indices corresponding to the physical systems in 1D. Analogously, the rows $2, 3, \ldots, N_v - 1$ can be considered as matrix product operators (MPO) [5],

$$U_k := \sum_{d_1, u_1 \ldots = 1}^{D^2} \mathrm{F}(E_{1,1}^{d_1,u_1}, \ldots, E_{1,N}^{d_N,u_N}) |d_1 \ldots d_N\rangle\langle u_1 \ldots u_N|.$$

We have $\langle\Psi|O|\Psi\rangle = \langle U_N|U_{N-1}\ldots U_2|U_1\rangle$.

The evaluation of expectation values poses a serious problem since the number of indices proliferate after each contraction. For example, the vector $|U_2\rangle := U_2|U_1\rangle$ can be written as the MPS (4a) but with the substitution

$$E_{1,n}^{d_n} \to \sum_{d_n=1}^{D^2} E_{1,n}^{d_n} \otimes E_{2,n}^{d'_n,d_n}. \tag{5}$$

This last tensor has more (right and left) indices than the original one. Thus, every time we apply the MPO U_k to a MPS $|U_{k-1}\rangle$ the number of indices increases, and thus the problem soon becomes intractable. Now we introduce a numerical algorithm inspired by DMRG to numerically determine $\mathrm{F}_2(E_{O_{h,c}})$ and to overcome this problem.

Given an unnormalized MPS $|\psi_A\rangle$ parameterized by $D \times D$ matrices $\{A_k^s\}$, the goal is to find another MPS $|\psi_B\rangle$, parameterized by $D_f \times D_f$ matrices $\{B_i^s\}$, where $D_f < D$ is a prescribed number. This has to be done such that $K := \||\psi_A\rangle - |\psi_B\rangle\|^2$ is minimal, i.e., such that that $|\psi_B\rangle$ gives the best approximation to $|\psi_A\rangle$. We have developed an algorithm that achieves this task in an iterative way. The key insight is that K is quadratic in all components of the matrices $\{B_k^s\}$, and hence if all these matrices are fixed except one of them (say B_j^s) K is quadratic in the components of B_j^s; the optimal choice for B_j^s thus amounts to solving a trivial system of linear equations. Having done that, one moves to the next site $j+1$, fixes all other ones and repeats the same procedure. After a few sweeps back and forth the optimal MPS is found. Note that the error in the approximation is exactly known and if it becomes too large one can always increase D_f; in all relevant situations we encountered the error could be made very small even with moderate D_f. The same reasoning holds for MPS defined with periodic instead of open boundary conditions. In this latter case considered here, one can further simplify the system of linear equations by performing a singular value decomposition of B_j^s and keeping only one of the unitary matrices at each step, analogously as one does in DMRG.

Thus, in order to evaluate an arbitrary expectation value we first determine the MPS $|\tilde{U}_2\rangle$ which is the closest to $U_2|U_1\rangle$ but with a fixed dimensions D_f of the corresponding matrices. Then, we determine $|\tilde{U}_3\rangle$, which is the closest to $U_3|\tilde{U}_2\rangle$, and continue in this vein until we finally determine $\langle\Psi|O|\Psi\rangle \simeq \langle U_N|\tilde{U}_{N-1}\rangle$. Interestingly enough, this method to calculate expectation values and to determine optimal approximations to MPS can be adapted to develop very efficient algorithms to determine the ground states of 2D Hamiltonians and the time evolution of PEPS by extending DMRG and the time evolution schemes to 2D.

Let us start with an algorithm to determine the ground state of a Hamiltonian with short range interactions on a square $N_h \times N_v$ lattice. The goal is to determine the PEPS (2) with a given dimension D which minimizes the energy. Following [9], the idea is to iteratively optimize the tensors $A_{h,c}^s$ one by one while fixing all the other ones. The crucial observation is the fact that the exact energy of $|\psi\rangle$ (and also its normalization) is a quadratic function of the components of the tensor $A_{\bar{h},\bar{c}}^s$ to be optimized, which we write as a vector x; hence the energy can be expressed in terms of an effective Hamiltonian:

$$E = \frac{x^\dagger \hat{H}_{eff} x}{x^\dagger \hat{N} x} \tag{6}$$

The denominator takes the normalization of the state into account. This expression can readily be minimized as it is equivalent to a generalized eigenvalue problem. It turns out that $\hat{H}_{eff}$ and $\hat{N}$ can be efficiently evaluated by the methods described above. In the case of $\hat{N}$, the MPS $|U_1\rangle$ (4a) constructed from $E_{\mathbb{1}_{h,1}}$ can be propagated up to the row $\bar{v} - 1$ with the technique outlined before. Similarly, the last row $\langle U_{N_v}|$ (4b) can be propagated up to row $\bar{v} + 1$. The tensors $E_{\mathbb{1}_{h\bar{v}}}$ can now be contracted with these two MPS from $h = 1..\bar{h} - 1$, and similarly from $h = N_h..\bar{h} + 1$. The remaining tensor has 4 (double) indices from which one can readily determine $\hat{N}$. $\hat{H}_{eff}$ can be determined in an analogous way, but here the procedure has to be repeated for every term in the Hamiltonian (i.e. in the order of $2N_hN_v$ times in the case of nearest neighbor interactions). Thus both $\hat{N}$ and $\hat{H}_{eff}$ can be calculated efficiently. Therefore the optimal $A_{\bar{h}\bar{v}}^s$ can be determined, and one can proceed with the following projector, iterating the procedure until convergence.

In a practical implementation one can save much time by storing appropriate tensors, implementing the algorithm in a parallel way, doing sparse tensor multiplications, and making use of quantum numbers and reflection symmetries. A more efficient variant can also be constructed by an iterative procedure which resembles the infinite-size DMRG-algorithm, where new rows are inserted in the middle of the lattice.

Let us next move to describe how time-evolution can be simulated on a PEPS. We will assume that the Hamiltonian only couples nearest neighbors, although more general settings can be considered. The simplest scheme would work by optimally mapping a given PEPS to another PEPS after an infinitesimal time-step $\mathbb{1} - iH\delta t$. It can readily be checked that, up to first order of δt, the action of this operator is to map a TPS with auxiliary dimension D onto a new TPS with dimension of the auxiliary bonds nD; here n represents the minimal number

of terms needed to express the couplings as tensor products of local operators plus 1 (e.g. $n = 2$ for the Ising interaction and $n = 4$ for the Heisenberg interaction). In analogy to the method introduced above for MPS, one can approximate this new PEPS with another one having again bonds of auxiliary dimension D. The algorithm to achieve this is a direct generalization of the method introduced to reduce the D of MPS: again several sweeps over all projectors have to be done, and the only difference is that at each step correlation functions of a PEPS have to be calculated instead of correlations function of a MPS. This can be done using the methods introduced before. Of course there are again many possibilities to boost the accuracy and to reduce the computational cost of such an implementation, such as using the Trotter decomposition as in [3] and then using the sweeps to optimize the state. This algorithm can also be used to solve finite temperature or dissipation problems by extending the ideas of [4] and [5].

Let us now illustrate our methods with an example. We consider a 2D lattice of spin 1/2-particles where nearest neighbors interact via the antiferromagnetic Heisenberg interaction with coupling constant $J = 1$. We use the time–evolution algorithm for evolving the PEPS in imaginary time; in this way we illustrate both the fact that the new formalism allows us to find ground states as well as to describe time-evolution. We implemented the algorithm as follows: we start with a completely separable state $|\psi_0\rangle$ in which the spins are rotated by an angle $\pi/16$ with respect to the previous one, and which can trivially be written as a PEPS. Using the Trotter decomposition, we divide each time step into 4 parts in which each spin is only interacting with one neighbor; as we are considering the Heisenberg interaction, the dimension D between the 2 interacting spins gets multiplied by a factor of 4. Let us parameterize this new PEPS with the corresponding tensors $B^s_{h,v}$. After each of these substeps, we want to reduce the dimension again to the original one giving rise to the PEPS $C^s_{h,v}$ that optimally approximates the exact $B^s_{h,v}$. This is done in an iterative way, row by row, until convergence. Fixing all rows but one, the problem of finding the optimal projectors in this row is equivalent to the problem of approximating a MPS with another one with lower dimension (the physical dimension of the MPS is the product of the bonds going up and down), which can on itself done in an iterative way as outlined above. Note that the computational cost of the algorithm is polynomial in N and D.

We have first considered a 4×4 lattice on which the imaginary time evolution can be determined exactly. In Fig. 2, we plotted the exact evolution versus the one where the evolution is approximated variationally within the PEPS with bonds of dimension $D = 2, 3$ ($D = 4$ cannot be distinguished from the exact result). We used the same Trotter approximation for the exact and variational simulations with $\delta t = -3i/100$. It is remarkable that

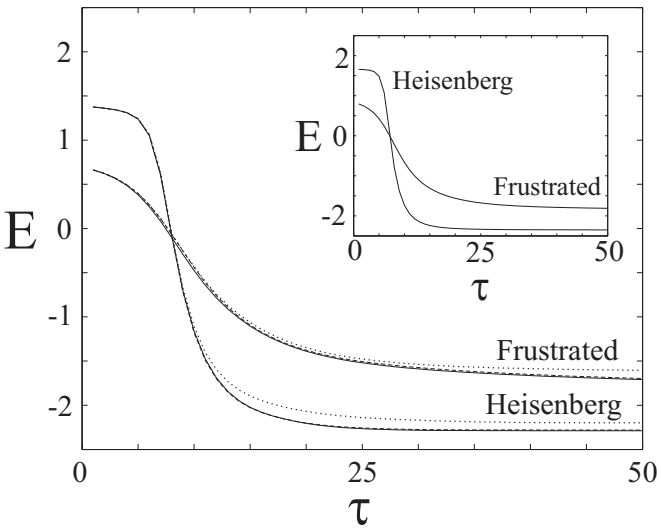

FIG. 2: Imaginary time evolution with the Heisenberg and a frustrated Heisenberg interaction on a 4×4 lattice, and $D = 2, D_f = 16$ (dotted) and $D = 3, D_f = 35$ (dashed); the $D = 3$ results are almost indistinguishable from the exact ones (full line). The insert presents the evolution for $D = 2$ on a 10×10 lattice.

even for $D = 3$ we obtain a very good approximations, both regarding time evolution and ground state energy. The algorithm clearly converges to the ground state, and the difference between the exact ground state energy and the one obtained with our scalable algorithm rapidly decreases with D[17]; more specifically, $1 - E_{var}/E_{exact}$ is given by $.35, .02; .004; 0.0008$ for $D = 1, 2; 3; 4$ (note that the trivial situation $D = 1$ corresponds to the Néel state). We also repeated the same simulation but with a frustrated Heisenberg Hamiltonian, obtained by making 1 out of every 4 interactions on each spin ferromagnetic instead of antiferromagnetic. Again very good agreement with the exact results is obtained; note that the energy converges more slowly due to the fact that the energy gap is smaller. The insert of Fig. (2) presents some simulation results for the imaginary time evolution for a square 10×10 lattice for both the Heisenberg antiferromagnet and the frustrated case. The convergence is again very fast, and increasing D from 2 to 3 (not shown in the plot) allows us to find a better value for the energy of the ground state. Note that we can easily handle larger systems and, using the appropriate numerical techniques, eventually increase the value of D.

In conclusion, we have introduced the class of PEPS and showed how they arise naturally in the context of constructing variational ground states for spin Hamiltonians on higher dimensional lattices. We presented an efficient algorithm for calculating correlation functions, which leads to scalable variational methods for finding ground states and for describing their real or imaginary time evolution. Interestingly, the methods described also

apply in the case of different geometries, of evolution in the presence of dissipation, and for finding finite-T states. It is also possible to identify quite generic classes of PEPS for which 2-point correlation functions can be calculated analytically [18]. We also note that the concept of PEPS could be very useful for the description of 2-dimensional transport problems, as the PEPS generalize the matrix product states which proved to be very useful in the 1-D case [19].

We thank M. A. Martin-Delgado for his insights on DMRG and MPS. Work supported by the DFG (SFB 631), european projects (IST and RTN), and the Kompetenznetzwerk der Bayerischen Staatsregierung Quanteninformation.

[1] I. Affleck *et al.*, Commun. Math. Phys. **115**, 477 (1988).
[2] S.R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[3] G. Vidal, Phys. Rev. Lett. 91, 147902 (2003); A. Daley *et al.*, J.Stat.Mech.: Theor.Exp. P04005 (2004); S.R. White and A.E. Feiguin, cond-mat/0403310.
[4] M. Zwolak and G. Vidal, cond-mat/0406440.
[5] F. Verstraete, J.J. Garcia-Ripoll and J. I. Cirac, cond-mat/0406426.
[6] M. Fannes, B. Nachtergaele and R.F. Werner, Comm. Math. Phys. **144**, 443 (1992).
[7] S. Ostlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995).
[8] J. Dukelsky *et al.*, Europhys. Lett. **43**, 457 (1997).
[9] F. Verstraete, D. Porras and J.I. Cirac, cond-mat/0404706.
[10] D.M. Ceperley and B.J. Alder, Phys. Rev. Lett. **45**, 566 (1980).
[11] Y. Hieida, K. Okunishi and Y. Akutsu, New J. Phys. **1**, 7 (1999); K. Okunishi and T. Nishino, Prog. Teor. Phys. **103**, 541 (2000); T. Nishino *et al.*, Nucl. Phys. B **575**, 504 (2000); Y. Nishio *et al.*, cond-mat/0401115.
[12] H. Niggeman, A. Klümper and J. Zittartz, Z. Phys. B **104**, 103 (1997).
[13] M.A. Martín-Delgado, M. Roncaglia and G. Sierra, Phys. Rev. B **64**, 075117 (2001).
[14] F. Verstraete and J.I. Cirac, quant-ph/0311130.
[15] G. Vidal *et al.*, Phys.Rev.Lett. **90**, 227902 (2003).
[16] S. Liang and H. Pang, Phys. Rev. B **49**, 9214 (1994); S.R. White, Phys. Rev. Lett. **77**, 3633 (1996); T. Xiang, J. Lou, and Z. Su, Phys. Rev. B **64**, 104414 (2001).
[17] The number of variational parameters scales as D^4, whereas for 1D MPS it does as D^2. Thus, modest values of D already allow us to approximate the local 2-body density operators (and hence the energy) to a good accuracy.
[18] In Preparation
[19] B. Derrida *et al.*, J. Phys. A: Math. Gen. **26**, 1493 (1993).